I checked the code of Wing-Fai today, which treats the photo-dissociation and photo-ionisation rates with detailed cross sections and the Jnu from spline-interpolated band RT-results. It's good work and seems well tested. I trust it more than anything else we have used so far.

Nevertheless, I found some small bugs and applied some cosmetic changes that hopefully make the code easier to understand. The "bugs" concern the assignment of photo-cross sections to the actual reaction numbers in ProDiMo ("P3"-type), some accelerations (photoindex) and more tests and warnings. There were also some errors in the Ly-alpha cross-section assignments (currently unused).

I checked the very old (2-stream UMIST with chifac), old (generic cross section sig = sig0*exp(-(lam-lam0)^2/(0.1*lam0)^2) with fitted sig0,lam0 to UMIST data, and new rates. Differences are as large as 10^6 for Herbig-disk even in the un-attenuated case (!), i.e. at ProDiMo grid point (1,1).

This reflects the "much redder" incident stellar intensities as compared to a Draine-field. It just makes a huge difference whether the cross-section is at 100nm or 200nm, because the star is much dimmer at 100nm. Might be less significant for TTauri with UV excess. The differences in the middle of the disk with scattering can be even more substantial.

During my "verification tests", I had some thoughts which I would like to share with you:

- there are additional output lines in ChemInit.log. Take a look! As expected, there are reactions for which no cross-sections are available in Leiden's database - these are treated with the "old" method. There are also cross-sections available for reactions not found in UMIST or Reaction.in. These are presently ignored. One could add these reactions if reactant and all products are present.

- try to uncomment "call test_photoreactions" in init_photoreactions()! This makes detailed tests for a Draine-field, 10000K-bb, and 4000K-bb rates in comparison to the values listed on the Leiden webpage. The output shows a "*" for >20% deviation.

  press <ENTER> after each block

  There are some deviations for H2O -> H2 + O and NH3 -> NH + H2, due to complicated branching ratio differences, which should only affect this test but not the main program.

- one side result is that *** UMIST ALPHA IS FOR 4pi DRAINE IRRADIATION - NOT 2pi ***, so the factor 2 in Paper I is wrong. Because we can re-calculate alpha now, and it fits in many cases. This is an issue! In particular for H2, see below.

  ==> I have hence eliminated the *2 in rate_coeff !!! <==

  IS THAT OK ???

- CO (new treatment) versus CODIS-routine gives the same result within 2% in the unattenuated case!

- The way we calculate photo-rates now,
  cross-section * SplineInterPol(RT-Jnu),
  disregards anti-correclations between line-dominated input spectrum and line-dominated cross section. A better idea would be to scale the

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  I^inc(nu)-"band-patterns" with band-mean RT-results, and then do the
  integral. ToDo.

- The most important photo-process H2 + hv -> H + H has no Leiden-data!
  Thus it is still treated according to the "old" treatment, e.g. with
  generic cross-section (before self-shielding). Analysis gives

  sig0 = 1.2E-18 cm^2, lam0=114nm, dlam=11nm

  sig = sig0 * exp((lam-lam0)^2/dlam^2)

  It results in unshielded 4pi-Draine rate of 4.2E-11 1/s

  DO YOU THINK THIS IS A REASONABLE ASSUMPTION ???


Cheers,

  Peter
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